

All Maximally Entangled Four Qubits States

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We find an operational interpretation for the 4-tangle as a type of residual entanglement, somewhat similar to the interpretation of the 3-tangle. Using this remarkable interpretation, we are able to find the class of maximally entangled four-qubits states which is characterized by four real parameters. The states in the class are maximally entangled in the sense that their average bipartite entanglement with respect to all possible bi-partite cuts is maximal. We show that while all the states in the class maximize the average tangle, there are only few states in the class that maximize the average Tsallis or Renyi α -entropy of entanglement. Quite remarkably, we find that up to local unitaries, there exists two unique states, one maximizing the average α -Tsallis entropy of entanglement for *all* $\alpha \geq 2$, while the other maximizing it for all $0 < \alpha \leq 2$ (including the von-Neumann case of $\alpha = 1$). Furthermore, among the maximally entangled four qubits states, there are only 3 maximally entangled states that have the property that for 2, out of the 3 bipartite cuts consisting of 2-qubits versus 2-qubits, the entanglement is 2 ebits and for the remaining bipartite cut the entanglement between the two groups of two qubits is 1 ebit. The unique 3 maximally entangled states are the 3 cluster states that are related by a swap operator. We also show that the cluster states are the only states (up to local unitaries) that maximize the average α -Renyi entropy of entanglement for *all* $\alpha \geq 2$.

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I. INTRODUCTION

Entanglement lies at the heart of quantum physics. It was clear immediately after the discovery of quantum mechanics that entanglement is not “one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought” [1]. Nevertheless, it was not until recently, that entanglement, besides of being interesting from a fundamental point of view, was also recognized as a valuable resource for two-party communication tasks such as teleportation [2] and superdense coding [3]. With the emergence of quantum information science in recent years, much effort has been given to the study of bipartite entanglement [4]; in particular, to its characterization, manipulation and quantification [5]. It was realized that maximally entangled states are the most desirable resources for many quantum information processing (QIP) tasks. While two-party entanglement was very well studied, entanglement in multi-party systems is far less understood, and even the identification of maximally entangled states in multi-party systems is a highly non-trivial task.

The understanding of highly entangled multi-qubit states is crucial for the implementation of many QIP tasks in quantum networks. Highly entangled multi-qubit states, such as the cluster states or graph states, are the key resource of one-way or measurement based quantum computer [6], and as such raised enormous interest

in the QIP community. Even experimental realizations of one-way quantum computing with four-qubit cluster states has been demonstrated successfully [7]. Highly entangled multi-qubit states are also the key ingredients of various quantum error correction codes and quantum communication protocols [8–10]. However, unlike bipartite entanglement, very little is known about the characterization of entanglement in multi-qubits systems.

The complexity in the characterization of entanglement in multi-partite systems can already be seen in the fact that for 3 qubits there are essentially two types of genuine 3-partite entanglement and even the notion of maximally entangled states is not unique [11]. One can think of both the GHZ-state, $|\text{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$, and the W-state $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ as two types of maximally entangled states, that are not related by stochastic local operations and classical communication (SLOCC). Nevertheless, in the case of 3-qubits, one can single out the GHZ-state as the unique maximally entangled state for the following two reasons. First, the GHZ class (i.e. the set of states that can be obtained from the GHZ state by SLOCC) is dense in the space of 3-qubits and therefore the W-class is of measure zero. This means that by LOCC it is possible to convert the GHZ state to a state that is arbitrarily close to the W-state, but the W-state can not be converted (not even by SLOCC) to a state that is close to the GHZ-state. Second, the GHZ-state is the only 3-qubit state with the property that the bipartite entanglement between any one qubit and the other two qubits is maximal; that is, the reduced density matrix obtained after the tracing out of any two qubits is proportional to

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the identity.

Similarly, for n -qubits one can define maximally entangled states as states with the property that the reduced density matrix obtained after the tracing out of any k qubits, with $n/2 \leq k \leq n-1$, is proportional to the identity. For example, the codeword states of the 5-qubits error correcting codes are maximally entangled [12]. However, as we show below, for four qubits such states do not exist. It is also known [13] that maximally entangled states exist for $n = 6$ and do not exist for $n \geq 8$. To the authors knowledge, the case of $n = 7$ is unknown.

In this paper we find an operational interpretation of the 4-tangle which enable us to characterize all maximally entangled four-qubits states. We define a state to be maximally entangled if its average bipartite entanglement with respect to all possible bi-partite cuts is maximal (e.g. see [14, 15] and references therein). More precisely, we divide the four qubits into two groups, each consisting of two qubits, and calculate the pure bipartite entanglement between the two groups of qubits. We then find the class of all states that maximize the average entanglement of the $3 = \binom{4}{2}/2$ such (inequivalent) bi-partite cuts. We find that when we take the measure of bipartite entanglement to be the tangle, there is a 4-real parameter class of states \mathcal{M} that maximize the average tangle. However, when we take the measure to be the entropy of entanglement, or the Tsallis and Renyi α -entropy of entanglement, we get that up to local unitary there are only two states that maximize the average α -entropy of entanglement. Quite remarkably, we find that up to local unitaries the state

$$|L\rangle = \frac{1}{\sqrt{3}} [u_0 + \omega u_1 + \omega^2 u_2] , \quad (1)$$

where $\omega = e^{i2\pi/3}$,

$$\begin{aligned} u_0 &\equiv |\phi^+\rangle|\phi^+\rangle , & u_1 &\equiv |\phi^-\rangle|\phi^-\rangle \\ u_2 &\equiv |\psi^+\rangle|\psi^+\rangle , & u_3 &\equiv |\psi^-\rangle|\psi^-\rangle \end{aligned}$$

and $|\phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ and $|\psi^\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$, is the only state that maximize the average Tsallis α -entropy of entanglement for *all* $\alpha > 2$ (see Fig. 1). Interesting properties of the state $|L\rangle$ have been discussed in [14, 16].

On the other hand, we show that the state

$$|M\rangle = \frac{i}{\sqrt{2}} u_0 + \frac{1}{\sqrt{6}} [u_1 + u_2 + u_3] \quad (2)$$

is the only state that maximize the Tsallis α -entropy of entanglement for all $0 < \alpha < 2$. Ten years ago the state $|M\rangle$ was conjectured to maximize the entropy of entanglement [17]. More recently, it was proved that locally it is indeed maximally entangled [18]. In Fig. 1 we draw a graph of the average Tsallis α -entropy of entanglement as a function of α for the states $|M\rangle$ and $|L\rangle$.

In addition, among the maximally entangled four qubits states, we identify 3 ultimate maximally entangled states that have the property that for 2, out of the

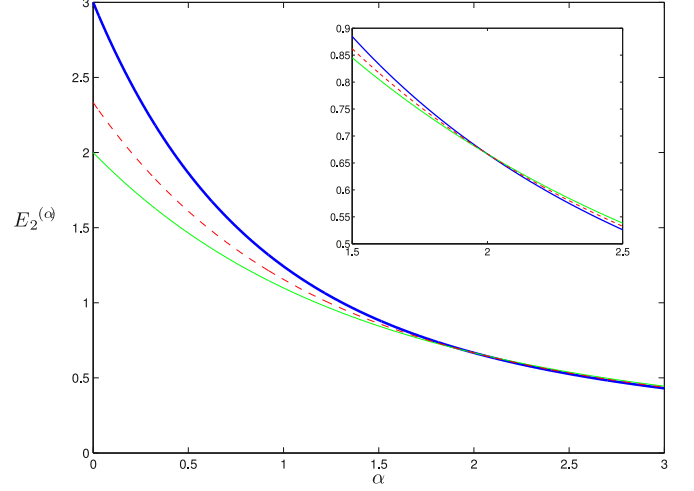


FIG. 1: A graph of the average Tsallis α -entropy of entanglement as a function of α . The blue line corresponds to the state $|M\rangle$, the green line to the state $|L\rangle$, and the dashed red line to the cluster states. Like the cluster states, the graph for any maximally entangled state in \mathcal{M} is between the blue and green lines.

3 bipartite cuts, the entanglement is 2 ebits and for the last bipartite cut the entanglement between the groups of two qubits is 1 ebit. The unique 3 maximally entangled states are the 3 cluster states that are related by a swap operator (but not by SLOCC):

$$|C_1\rangle = \frac{1}{2} (|0000\rangle + |1100\rangle + |0011\rangle - |1111\rangle) \quad (3)$$

$$|C_2\rangle = \frac{1}{2} (|0000\rangle + |0110\rangle + |1001\rangle - |1111\rangle) \quad (4)$$

$$|C_3\rangle = \frac{1}{2} (|0000\rangle + |1010\rangle + |0101\rangle - |1111\rangle) \quad (5)$$

We show that these cluster states are the only states that maximize the Renyi α -entropy of entanglement for all $\alpha \geq 2$.

This paper is organized as follows, in section (II) we discuss the generic class of four qubits states, consisting of an uncountable number of SLOCC-inequivalent classes. In section (III) we find an operational interpretation of the 4-tangle and discover a four real parameter class of all four qubits states that maximize the average tangle. We then use this result in section (IV) to find maximally entangled states with respect to other measures of entanglement, such as the Tsallis and Renyi α -entropy of entanglement. In section (V) we discuss more maximally entangled four qubits states. We end in section (VI) with a summary, conclusions and a discussion on the extension of the results presented here in higher dimensions.

II. UNCOUNTABLE NUMBER OF FOUR QUBITS SLOCC-INEQUIVALENT CLASSES

In [21] it was argued that 4-qubits pure states can be classified into nine groups of states. One of these nine groups is called the generic class as with the action of SLOCC it is dense in the space of 4-qubits $\mathcal{H}_4 \equiv \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. The generic class is given by

$$\mathcal{A} \equiv \left\{ z_0 u_0 + z_1 u_1 + z_2 u_2 + z_3 u_3 \mid z_0, z_1, z_2, z_3 \in \mathbb{C} \right\}.$$

In [20, 21] it has been shown that all the states that are connected to the class \mathcal{A} by SLOCC form a dense set of states. That is, the class of states $G\mathcal{A}$, where $G \equiv \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C})$, is dense in \mathcal{H}_4 . In the following we discuss several properties of the generic class that will be very useful for our theorems in the next sections.

For $k = 0, 1, 2, 3$, we denote by $|k\rangle\rangle \equiv |ij\rangle$, with $i, j = 0, 1$, a state of two qubits, such that ij is the binary representation of k . Hence, any $|\psi\rangle \in \mathcal{H}_4$ can be written as

$$|\psi\rangle = \sum_{k=0}^3 \sum_{k'=0}^3 T_{kk'} |k\rangle\rangle |k'\rangle\rangle, \quad (6)$$

where $\{|k\rangle\rangle\}$ is the computational basis of qubits 1 and 2, and $\{|k'\rangle\rangle\}$ is the computational basis of qubits 3 and 4. With these notations we define the following four quantities:

Definition 1. Let $|\psi\rangle \in \mathcal{H}_4$. Then,

$$\mathcal{E}_m(|\psi\rangle) \equiv \begin{cases} \text{Det}[T_\psi] & \text{if } m = 0 \\ \text{Tr}[(T_\psi J T_\psi^T J)^m] & \text{if } m = 1, 2, 3 \end{cases}$$

where T_ψ is the 4×4 matrix whose components $T_{kk'}$ are defined in Eq. (6), and

$$J \equiv \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

The four polynomials defined above take a simple form on \mathcal{A} . If $|\psi\rangle = \sum_{j=0}^3 z_j u_j$ then

$$\mathcal{E}_m(|\psi\rangle) = \begin{cases} z_0 z_1 z_2 z_3 & \text{if } m = 0 \\ z_0^{2m} + z_1^{2m} + z_2^{2m} + z_3^{2m} & \text{if } m = 1, 2, 3 \end{cases}$$

In [20, 21] it has been shown that these four polynomials are invariant under the action of the group $G \equiv \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C}) \otimes \text{SL}(2, \mathbb{C})$. That is, if $g \in G$ and $|\psi\rangle \in \mathcal{H}_4$ then $\mathcal{E}_m(g|\psi\rangle) = \mathcal{E}_m(|\psi\rangle)$ for all $m = 0, 1, 2, 3$. Other polynomials that corresponds to true ‘tangles’ have been considered for example in [16]. As discussed in [21, 22], one of the consequences of this property is that the four functions $f_m \equiv |\mathcal{E}_m|^{1/m}$ ($m = 1, 2, 3$) and $f_0 \equiv \sqrt{|\mathcal{E}_0|}$ are

entanglement monotones [34]. However, here we show that this property implies that almost all the states in \mathcal{A} are not related by SLOCC, which means that \mathcal{A} contains an uncountable number of SLOCC inequivalent classes of states.

Proposition 1. (c.f. [20, 22, 25]) Let $|\psi\rangle$ and $|\psi'\rangle$ be two normalized states in \mathcal{A} . Then, the transformation $|\psi\rangle \rightarrow |\psi'\rangle$ can be achieved by SLOCC only if $f_m(|\psi\rangle) = f_m(|\psi'\rangle)$ for all $m = 0, 1, 2, 3$.

Proof. Let $\psi \in \mathcal{A}$ be a normalized state and let $g \in G$. Then,

$$f_m\left(\frac{g\psi}{\|g\psi\|}\right) = \frac{f_m(g\psi)}{\|g\psi\|^2} = \frac{f_m(\psi)}{\|g\psi\|^2} \leq f_m(\psi),$$

where in the last inequality we used the fact that for $\psi \in \mathcal{A}$ and $g \in G$, $\|g\psi\| \geq \|\psi\| = 1$ (see Appendix A for the Kempf-Ness theorem [24]). \square

In the definition above \mathcal{E}_m is defined only for $m \leq 3$. The absolute value of the polynomials with higher values of m are also entanglement monotones, but they are in the algebra generated by these four polynomials and therefore do not contain any additional information about the entanglement of the states.

The proposition above implies that the class \mathcal{A} contains an uncountable number of states that are not connected by SLOCC transformation. More precisely, if $|\psi\rangle = \sum_{j=0}^3 z_j u_j$ and $|\psi'\rangle = \sum_{j=0}^3 z'_j u_j$, and there is no permutation σ such that $z_j = \pm z'_{\sigma(j)}$ for $j = 0, 1, 2, 3$ with an even number of $-$ signs, then the transformation $|\psi\rangle \rightarrow |\psi'\rangle$ can not be achieved by SLOCC. Moreover, from the proposition below it follows that on \mathcal{A} if two states are connected by SLOCC operation, then the transformation must be a local unitary.

Proposition 2. [20, 22, 25] Let $|\psi\rangle, |\psi'\rangle \in \mathcal{A}$. Then, the transformation $|\psi\rangle \rightarrow |\psi'\rangle$ can be achieved by a local unitary $U \in \text{SU}(2) \otimes \text{SU}(2) \otimes \text{SU}(2) \otimes \text{SU}(2)$ if and only if $\mathcal{E}_m(|\psi\rangle) = \mathcal{E}_m(|\psi'\rangle)$.

For the purpose of this work, we generalize the proposition above to include all local unitaries; that is, not only those in $\text{SU}(2) \otimes \text{SU}(2) \otimes \text{SU}(2) \otimes \text{SU}(2)$.

Proposition 3. Set

$$f_4 = |\mathcal{E}_1^2 - \mathcal{E}_0|^2, \quad f_5 = |\mathcal{E}_1^2 - \mathcal{E}_2|^2, \quad f_6 = |\mathcal{E}_1^3 - \mathcal{E}_3|^2.$$

Let $|\psi\rangle, |\psi'\rangle \in \mathcal{A}$. Then, the transformation $|\psi\rangle \rightarrow |\psi'\rangle$ can be achieved by a local unitary $U \in \text{U}(2) \otimes \text{U}(2) \otimes \text{U}(2) \otimes \text{U}(2)$ if and only if $f_m(|\psi\rangle) = f_m(|\psi'\rangle)$ for all integers $0 \leq m \leq 6$.

Proof. Note that the first 4 conditions (i.e. $m = 0, 1, 2, 3$) imply that

$$\begin{aligned} \mathcal{E}_0(\psi) &= a\mathcal{E}_0(\psi'), \quad \mathcal{E}_1(\psi) = b\mathcal{E}_1(\psi') \\ \mathcal{E}_2(\psi) &= c\mathcal{E}_2(\psi'), \quad \mathcal{E}_3(\psi) = d\mathcal{E}_3(\psi'), \end{aligned}$$

with $|a| = |b| = |c| = |d| = 1$. $f_4(\psi) = f_4(\psi')$ implies that $a = b^2$. Similarly, the condition on f_5 implies $c = b^2$, and the condition on f_6 implies $d = b^3$. Now, write $b = r^2$. We therefore have

$$\begin{aligned}\mathcal{E}_0(\psi) &= \mathcal{E}_0(r\psi') , \quad \mathcal{E}_1(\psi) = \mathcal{E}_1(r\psi') \\ \mathcal{E}_2(\psi) &= \mathcal{E}_2(r\psi') , \quad \mathcal{E}_3(\psi) = \mathcal{E}_3(r\psi') .\end{aligned}$$

Thus, from proposition 2, $|\psi\rangle$ and $r|\psi'\rangle$ are related by a local unitary in $SU(2) \otimes SU(2) \otimes SU(2) \otimes SU(2)$. The argument clearly can run backwards. \square

As we show now, among the 4 entanglement monotones f_m ($m = 0, 1, 2, 3$), the 4-qubits entanglement monotone f_1 is the only one that is invariant under any permutation of the 4-qubits. In fact, we find that this monotone is the 4-tangle.

A. The monotone $f_1 \equiv |\mathcal{E}_1|$ and the 4-tangle

Given a bipartite state $|\psi^{AB}\rangle \in \mathbb{C}^n \otimes \mathbb{C}^m$, the tangle (or the square of the I-concurrence) is defined by

$$\tau_{AB} \equiv \tau(|\psi^{AB}\rangle) = S_L(\rho_r) = 2(1 - \text{Tr}\rho_r^2) , \quad (7)$$

where $\rho_r = \text{Tr}_B|\psi^{AB}\rangle\langle\psi^{AB}|$ is the reduced density matrix, and S_L is the linear entropy.

For two qubits the tangle can be expressed as the square of the concurrence; that is, for $|\varphi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ the tangle is

$$\tau_{AB} = |\langle\varphi|\tilde{\varphi}\rangle|^2 \quad \text{where } |\tilde{\varphi}\rangle \equiv \sigma_y \otimes \sigma_y |\varphi^*\rangle ,$$

and σ_y is the second Pauli matrix. Note that the basis is chosen such that $\sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$, and if in this basis $|\varphi\rangle = \sum_{i,j} a_{ij}|ij\rangle$ then $|\varphi^*\rangle = \sum_{i,j} a_{ij}^*|ij\rangle$.

For mixed two qubits state ρ^{AB} , the tangle is defined in terms of the convex roof extension:

$$\tau_{AB} \equiv \tau(\rho^{AB}) \equiv \min \sum_i p_i \tau(|\psi_i\rangle) ,$$

where the minimum is taken over all the decompositions of the form $\rho^{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

In [26] it was shown that one can extend the definition of the 2-qubits tangle to 3-qubits. Given a 3-qubits pure state $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ the 3-tangle is defined by

$$\tau_{ABC} \equiv \tau(|\psi\rangle) \equiv \tau_{A(BC)} - \tau_{AB} - \tau_{AC} ,$$

where $\tau_{AB} \equiv \tau(\rho^{AB})$ (with $\rho^{AB} \equiv \text{Tr}_C|\psi\rangle\langle\psi|$), and $\tau_{A(BC)}$ is the tangle between the qubit system A and two qubits system BC. In [26] it was shown that the 3-tangle is non-negative and its square root has been proved to be an entanglement monotone in [22]. It was also shown [26] that it is symmetric under permutations of the three qubits A, B, and C. From its definition, the 3-tangle can be interpreted as the residual entanglement

between A and BC, that can not be accounted for by the entanglements of A and B, and A and C, separately.

The Wong-Christensen 4-tangle [27] is defined similarly. Let $|\psi\rangle \in \mathcal{H}_4 \equiv \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, the 4-tangle is defined by [27]

$$\tau_{ABCD} \equiv |\langle\psi|\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y|\psi^*\rangle|^2 .$$

In [27] the 4-tangle was shown to be an entanglement monotone and invariant under permutations. In the next section we will see that like the 3-tangle, the above 4-tangle can also be interpreted as a type of residual entanglement. Moreover, as we show now, the square of the monotone f_1 is the Wong-Christensen 4-tangle.

Proposition 4. *Let $|\psi\rangle \in \mathcal{H}_4$. Then,*

$$\tau_{ABCD}(|\psi\rangle) = |\mathcal{E}_1(|\psi\rangle)|^2 .$$

The above proposition follows directly from the fact that there is a single $SL(2, \mathbb{C})^{\otimes 4}$ invariant polynomial with homogeneous degree 2 [28]. Since both the 4-tangle and $|\mathcal{E}_1|^2$ have these properties they must be equal. In the proof below we show this equivalence by a direct calculation.

Proof. Denote $|\psi\rangle = \sqrt{p_0}|0\rangle|\phi^0\rangle + \sqrt{p_1}|1\rangle|\phi^1\rangle$, where $|\phi^j\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ with $j = 0, 1$ are three qubits orthonormal states. Also, denote

$$|\phi^j\rangle = \sum_{i \in \{0,1\}^3} a_i^{(j)} |i\rangle$$

for $j = 0, 1$. With this notations it is straightforward to show that both $\mathcal{E}_1(|\psi\rangle)$ and $\langle\tilde{\psi}|\psi\rangle$ equals

$$\begin{aligned}2\sqrt{p_0 p_1} & \left(a_{000}^{(0)} a_{111}^{(1)} + a_{110}^{(0)} a_{001}^{(1)} + a_{101}^{(0)} a_{010}^{(1)} + a_{011}^{(0)} a_{100}^{(1)} \right. \\ & \left. - a_{111}^{(0)} a_{000}^{(1)} - a_{001}^{(0)} a_{110}^{(1)} - a_{010}^{(0)} a_{101}^{(1)} - a_{100}^{(0)} a_{011}^{(1)} \right) .\end{aligned} \quad (8)$$

This completes the proof. \square

III. OPTIMIZING THE AVERAGE TANGLE

As a measure for pure bipartite entanglement we first take the tangle or the square of the I-concurrence (see Eq.(7)). Now, in four qubits there are 4 bipartite cuts consisting of one-qubit verses the rest 3 qubits and 3 bipartite cuts consisting of 2-qubits verses the rest 2 qubits. Denoting the four qubits by A, B, C, and D, we define

$$\tau_1 \equiv \frac{1}{4} (\tau_{A(BCD)} + \tau_{B(ACD)} + \tau_{C(ABD)} + \tau_{D(ABC)}) \quad (9)$$

$$\tau_2 \equiv \frac{1}{3} (\tau_{(AB)(CD)} + \tau_{(AC)(BD)} + \tau_{(AD)(BC)}) , \quad (10)$$

where $\tau_{A(BCD)}$, for example, is the tangle between qubit A and qubits B,C,D. Similarly, $\tau_{(AB)(CD)}$, for example, is the tangle between qubits A,B and qubits C,D. Note that

the maximum possible value for τ_1 is 1 and the maximum possible value for τ_2 is $3/2$ (since a maximally entangled 4×4 bipartite state has tangle $3/2$). However, it is argued now that no 4 qubit pure state can achieve this value for τ_2 .

In [19], it has been shown that

$$\tau_1 \leq \tau_2 \leq \frac{4}{3}\tau_1. \quad (11)$$

Hence, since τ_1 is bounded by 1, it follows that $\tau_2 \leq 4/3 < 3/2$. That is, there are no 4-qubit states for which all the 3 reduced density matrices, obtained by tracing out two qubits, are proportional to the identity. Moreover, from the inequality above, it follows that for states with $\tau_2 = 4/3$, τ_1 must be equal to 1. In the following theorem, we characterize all states with $\tau_1 = 1$.

Theorem 5. [21, 22] Let $|\psi\rangle \in \mathcal{H}_4 \equiv \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ be a normalized four qubit state. Then,

$$\tau_1(|\psi\rangle) = 1 \quad \text{if and only if} \quad |\psi\rangle \in \mathcal{A},$$

up to local unitary transformation.

A weaker version of the theorem above has been first pointed out in [21]. In [21] the authors argued that among all the states in \mathcal{GA} , only states in \mathcal{A} have $\tau_1 = 1$. A year later in [22] theorem 5 was fully proved. Nevertheless, for the purpose of completeness, we provide here a proof of Theorem 5 for all states in \mathcal{H}_4 , independently of the work in [21, 22].

Proof. Using the Kempf-Ness theorem [24] (see also Appendix A) applied to G (defined above) and the fact that \mathcal{GA} is the set of stable vectors [35], one can show that $\psi \in K\mathcal{A}$, with $K \equiv SU(2) \otimes SU(2) \otimes SU(2) \otimes SU(2)$, if and only if [25]

$$\langle \psi | X | \psi \rangle = 0, \quad (12)$$

for all X in $\text{Lie}(G)$. Note that $\text{Lie}(G)$ acting on \mathcal{H}_4 is the direct sum of the Lie algebras of $SL(2, \mathbb{C})$ acting on one tensor factor. Now, let ψ be a normalized state with $\tau_1(\psi) = 1$. Therefore, we can write $\psi = |0\rangle|\varphi_0\rangle + |1\rangle|\varphi_1\rangle$, with $\langle \varphi_0 | \varphi_0 \rangle = 1/2 = \langle \varphi_1 | \varphi_1 \rangle$ and $\langle \varphi_0 | \varphi_1 \rangle = 0$. Low, let

$$U \equiv \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

be a unitary matrix with $|a|^2 + |b|^2 = 1$. Then, if U_1 is U acting only in the first tensor factor we have

$$\langle \psi | U_1 | \psi \rangle = \frac{a + a^*}{2}.$$

Thus, the maximum value is attained at $U = I$. This implies that the condition in Eq.(12) is true for the part of the Lie algebra coming from the elements that act only on the first factor. The argument for the other factors is the same. \square

From the Eq. (11) it follows that among all the states with $\tau_1 = 1$, we have

$$1 \leq \tau_2 \leq \frac{4}{3}.$$

It is interesting to note that the 4-qubit GHZ state gives the minimum possible value for τ_2 . That is, it is the least entangled state among all the states with $\tau_1 = 1$. On the other hand, for all the 3 cluster states defined above, $\tau_2 = 4/3$. In fact, as we will see later, the cluster states are the *only* states that achieve the maximal value for τ_2 in such a way that 2 of the terms (i.e. tangles) appearing in the definition of τ_2 (see Eq. (10)) are equal to $3/2$ and one of the terms equals to 1.

From Theorem 5 and the inequality (11), it follows that only states in \mathcal{A} can maximize τ_2 . From the following theorem it also follows that states that maximize τ_2 must have zero 4-tangle.

Theorem 6. Let $\psi \in \mathcal{H}_4$ be a 4-qubits pure state and denote by $\tau_{ABCD}(\psi)$ its 4-tangle (defined above). Then,

$$\tau_2(\psi) = \frac{4\tau_1(\psi) - \tau_{ABCD}(\psi)}{3}.$$

Remark. The equation above can be written as $\tau_{ABCD} = 4\tau_1 - 3\tau_2$, where $4\tau_1$ can be interpreted as the total amount of entanglement in the system, whereas $3\tau_2$ can be interpreted as the total amount of entanglement shared among groups consisting of two qubits each. In this sense, the 4-tangle can be interpreted as the residual entanglement that can not be shared among the two qubits groups. Note that from the equation above it is obvious that the 4-tangle is invariant under permutations.

Proof. Following the same notations as in Proposition 4, we denote $|\psi\rangle = \sqrt{p_0}|0\rangle|\phi^0\rangle + \sqrt{p_1}|1\rangle|\phi^1\rangle$, where the 3-qubits states (qubits BCD), $|\phi^j\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ with $j = 0, 1$, are orthonormal. We also denote by \mathfrak{D}_X with $X \in \{B, C, D\}$ the *discriminant* of $|\psi\rangle$ [19]:

$$\mathfrak{D}_X \equiv \text{Tr}(\sigma_X^{00}\sigma_X^{11} - \sigma_X^{01}\sigma_X^{10}),$$

where

$$\sigma_X^{kk'} \equiv \text{Tr}_{\neq X} |\phi^k\rangle\langle\phi^{k'}| \quad \text{with } k, k' \in \{0, 1\}$$

and the trace is taken over all the remaining two qubits that are *not* the X qubit. The sum of the discriminants is denoted by $\mathfrak{D} \equiv \mathfrak{D}_B + \mathfrak{D}_C + \mathfrak{D}_D$.

With these notations the one-qubit reduced density matrices can be written as follows:

$$\begin{aligned} \rho^A &= \text{Tr}_{\neq A} |\psi\rangle\langle\psi| = p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1|, \\ \rho^X &= \text{Tr}_{\neq X} |\psi\rangle\langle\psi| = p_0\sigma_X^{00} + p_1\sigma_X^{11}. \end{aligned} \quad (13)$$

Similarly, the two-qubit reduced density matrices are given by

$$\rho^{AX} = \text{Tr}_{\neq AX} |\psi\rangle\langle\psi| = \sum_{k, k' \in \{0, 1\}} \sqrt{p_k p_{k'}} |k\rangle\langle k'| \otimes \sigma_X^{kk'}. \quad (14)$$

Substituting these reduced densities matrices in the expressions for the linear entropy gives

$$S_L(\rho^{AX}) - S_L(\rho^X) = 4p_0p_1\mathfrak{D}_X.$$

Since $S_L(\rho^A) = 4p_0p_1$, summing over X gives

$$4\tau_1 - 3\tau_2 = 4p_0p_1(1 - \mathfrak{D}).$$

Now, if we denote

$$|\phi^k\rangle = \sum_{i \in \{0,1\}^3} a_i^{(k)} |i\rangle$$

for $k = 0, 1$, then a straightforward calculation (see Eq.(3.38) in [19]) gives

$$\mathfrak{D} = 1 - \left| a_{000}^{(0)}a_{111}^{(1)} + a_{110}^{(0)}a_{001}^{(1)} + a_{101}^{(0)}a_{010}^{(1)} + a_{011}^{(0)}a_{100}^{(1)} - a_{111}^{(0)}a_{000}^{(1)} - a_{001}^{(0)}a_{110}^{(1)} - a_{010}^{(0)}a_{101}^{(1)} - a_{100}^{(0)}a_{011}^{(1)} \right|^2. \quad (15)$$

A comparison of this expression with the one given in Eq.(8) implies that $4\tau_1 - 3\tau_2 = \tau_{ABCD}$. \square

From Theorem 5 and Theorem 6, we have the following corollary.

Corollary 7. *A normalized state $|\psi\rangle \in \mathcal{H}_4$ is maximally entangled (i.e. $\tau_2(|\psi\rangle) = 4/3$) if and only if up to local unitary $|\psi\rangle \in \mathcal{M}$, where \mathcal{M} is the set of states in \mathcal{A} with zero 4-tangle.*

A state $\psi = \sum_{j=0}^3 z_j u_j$ in \mathcal{A} depends on four complex parameters z_j ($j = 0, 1, 2, 3$). The condition that the 4-tangle $\tau_{ABCD}(\psi) = |\sum_{j=0}^3 z_j^2|^2 = 0$ implies that the states in the maximally entangled class \mathcal{M} are characterized by 4 *real* parameters since we also have the normalization condition and we ignore the global phase. If we write $z_j = \sqrt{p_j}e^{i\theta_j}$ in its polar form (with non-negative p_j and $\theta_j \in [0, 2\pi]$) we can characterize the class \mathcal{M} as follows:

$$\mathcal{M} = \left\{ \sum_{j=0}^3 \sqrt{p_j} e^{i\theta_j} u_j \mid \sum_{j=0}^3 p_j = 1, \sum_{j=0}^3 p_j e^{2i\theta_j} = 0 \right\}. \quad (16)$$

Minimization of τ_2

From theorem 6, it also follows that the states in \mathcal{A} with the minimum possible value $\tau_2 = 1$, can be characterized as follows. Denote by \mathcal{T}_{\min} the class of all such states. Then,

$$\begin{aligned} \mathcal{T}_{\min} &\equiv \left\{ \psi \in \mathcal{A} \mid \tau_2(\psi) = 1 \right\} \\ &= \left\{ \sum_{j=0}^3 x_j u_j \mid \sum_{j=0}^3 x_j^2 = 1, x_j \in \mathbb{R} \right\} \end{aligned} \quad (17)$$

Note that the four qubits GHZ state belongs to \mathcal{T}_{\min} . In this sense, the GHZ state is a state in \mathcal{A} with the least amount of entanglement.

IV. DIFFERENT MEASURES OF ENTANGLEMENT

Up to now we took the measure in Eqs.(9,10) to be the tangle, which is given in terms of the linear entropy. The measures of entanglement that we consider in this section are Renyi entropy of entanglement and Tsallis entropy of entanglement. We denote these measures by $E_R^{(\alpha)}$ and $E_T^{(\alpha)}$, respectively. These bipartite measures of entanglement are defined as follows. Given a bipartite state $|\psi^{AB}\rangle \in \mathbb{C}^n \otimes \mathbb{C}^m$, the entanglements $E_R^{(\alpha)}$ and $E_T^{(\alpha)}$, measured by the Renyi and Tsallis entropies, are given by

$$\begin{aligned} E_R^{(\alpha)}(|\psi^{AB}\rangle) &\equiv \frac{1}{1-\alpha} \log \text{Tr} \rho_r^\alpha \\ E_T^{(\alpha)}(|\psi^{AB}\rangle) &\equiv \frac{1}{1-\alpha} (\text{Tr} \rho_r^\alpha - 1) \end{aligned}$$

where $\rho_r = \text{Tr}_B |\psi^{AB}\rangle \langle \psi^{AB}|$ is the reduced density matrix and the log is base 2. Note that both Renyi and Tsallis entropies approach the von-Neumann entropy in the limit $\alpha \rightarrow 1$. The Tsallis entropy is concave (see for example [29]) and therefore $E_T^{(\alpha)}$ is an ensemble entanglement monotone (i.e. non-increasing on average under LOCC). The Renyi entropy is also concave for $0 < \alpha \leq 1$, but only Shur concave for $\alpha > 1$ [30]. Hence, for $\alpha > 1$, $E_R^{(\alpha)}$ is only a deterministic monotone (i.e. non-increasing under deterministic LOCC). Nevertheless, unlike the Tsallis α -entropy of entanglement with $\alpha \neq 1$, the Renyi α -entropy of entanglement is normalized nicely so that it is equal $\log d$ for maximally entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$.

Similar to the definition of the average tangles (9,10), we define the average α -entropy of entanglement of four qubits states as follows:

$$E_1^{(\alpha)} \equiv \frac{1}{4} \left(E_{A(BCD)}^{(\alpha)} + E_{B(ACD)}^{(\alpha)} + E_{C(ABD)}^{(\alpha)} + E_{D(ABC)}^{(\alpha)} \right) \quad (18)$$

$$E_2^{(\alpha)} \equiv \frac{1}{3} \left(E_{(AB)(CD)}^{(\alpha)} + E_{(AC)(BD)}^{(\alpha)} + E_{(AD)(BC)}^{(\alpha)} \right), \quad (19)$$

where $E_{A(BCD)}^{(\alpha)}$, for example, is the Tsallis or Renyi α -entropy of entanglement between qubit A and qubits B,C,D, where it will be clear from the context if we mean Renyi or Tsallis. Note that due to Eq.(11) the maximum value of $E_2^{(\alpha)}$ cannot be 2 ebits (i.e. the same value as the the value for two bell states).

From Theorem 5 we know that $E_1^{(\alpha)}(|\psi\rangle) = 1$ iff $|\psi\rangle \in \mathcal{A}$. However, for the general measures of entanglement we do not have an equation analog to Eq. (11) and therefore, can not argue that if $|\psi\rangle$ maximize $E_2^{(\alpha)}$ then it must maximize $E_1^{(\alpha)}$. Nevertheless, we will see that for the average α -entropy of entanglement with $\alpha \geq 2$ this is indeed the case [36].

In order to optimize $E_2^{(\alpha)}$, we first prove the following theorem.

Theorem 8. *Let ρ be a 4×4 normalized density matrix with eigenvalues $\lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3$. Let $S_L(\rho) = \tau$ and denote $x(\tau) = \sqrt{1 - \frac{2}{3}\tau}$ and $y(\tau) = \sqrt{1 - \frac{3}{4}\tau}$. The maximum (minimum) possible value of either Tsallis or Renyi entropies with $0 < \alpha < 2$ ($\alpha > 2$) is obtained if and only if $\{\lambda_i\}$ is given by*

$$\left\{ \frac{1+3x(\tau)}{4}, \frac{1-x(\tau)}{4}, \frac{1-x(\tau)}{4}, \frac{1-x(\tau)}{4} \right\} \quad (20)$$

The minimum (maximum) possible value of Tsallis or Renyi entropies with $0 < \alpha < 2$ ($\alpha > 2$) is obtained if and only if the set $\{\lambda_i\}$ is given by

$$\begin{aligned} & \left\{ \frac{1+x(\tau)}{4}, \frac{1+x(\tau)}{4}, \frac{1+x(\tau)}{4}, \frac{1-3x(\tau)}{4} \right\} \quad \left(\frac{4}{3} \leq \tau \leq \frac{3}{2} \right) \\ & \left\{ \frac{1+y(\tau)}{3}, \frac{1+y(\tau)}{3}, \frac{1-2y(\tau)}{3}, 0 \right\} \quad (1 \leq \tau \leq \frac{4}{3}) \\ & \left\{ \frac{1+\sqrt{1-\tau}}{2}, \frac{1-\sqrt{1-\tau}}{2}, 0, 0 \right\} \quad (0 \leq \tau \leq 1) \end{aligned} \quad (21)$$

One direction of theorem 8 has been proven in [31]. To complete the proof of theorem 8, we show in Appendix B that the Renyi and Tsallis entropies obtain there extremum values *only* for the sets of eigenvalues that appear in the theorem.

A. The state $|L\rangle$

In this section we show that the state $|L\rangle$ in Eq. (1) has the remarkable property that it *maximizes* the average Tsallis entropy of entanglement $E_2^{(\alpha)}$ for *all* $\alpha \geq 2$. In addition, among all the states in \mathcal{M} , the state $|L\rangle$ *minimizes* $E_2^{(\alpha)}$ for *all* $0 \leq \alpha \leq 2$.

Theorem 9. (a) *Let $\psi \in \mathcal{H}_4$. Then,*

$$E_2^{(\alpha)}(\psi) \leq E_2^{(\alpha)}(|L\rangle) \text{ for all } \alpha > 2$$

with equality if and only if up to local unitaries $\psi = |L\rangle$.

(b) *Let $\psi \in \mathcal{M}$. Then,*

$$E_2^{(\alpha)}(\psi) \geq E_2^{(\alpha)}(|L\rangle) \text{ for all } 0 < \alpha < 2$$

with equality if and only if up to local unitaries $\psi = |L\rangle$.

Proof. Let $\tilde{E}_{\max}^{(\alpha)}(t)$ and $\tilde{E}_{\min}^{(\alpha)}(t)$ be, respectively, the maximum and minimum values $E_T^{(\alpha)}(\psi)$ can take among all normalized bipartite states $\psi \in \mathbb{C}^4 \otimes \mathbb{C}^4$ with tangle $\tau(\psi) = t$. Further, let $f_{\max}^{(\alpha)}(t_1, t_2, t_3) \equiv 1/3 \sum_{k=1}^3 \tilde{E}_{\max}^{(\alpha)}(t_k)$ and $f_{\min}^{(\alpha)}(t_1, t_2, t_3) \equiv 1/3 \sum_{k=1}^3 \tilde{E}_{\min}^{(\alpha)}(t_k)$. Thus, for a 4

qubit normalized state $|\psi\rangle \in \mathcal{H}_4$, with $\tau_{(12)(34)} = t_1$, $\tau_{(13)(24)} = t_2$, and $\tau_{(14)(32)} = t_3$,

$$f_{\min}^{(\alpha)}(t_1, t_2, t_3) \leq E_2^{(\alpha)}(|\psi\rangle) \leq f_{\max}^{(\alpha)}(t_1, t_2, t_3). \quad (22)$$

From theorem 8 and the definition of Tsallis entropy it follows that for $\alpha > 2$

$$\tilde{E}_{\max}^{(\alpha)}(t) = \frac{1}{\alpha-1} \times \begin{cases} \left[1 - \frac{3(1+x)^\alpha}{4^\alpha} - \frac{(1-3x)^\alpha}{4^\alpha} \right] & \text{for } \frac{4}{3} \leq t \leq \frac{3}{2} \\ \left[1 - \frac{2(1+y)^\alpha}{3^\alpha} - \frac{(1-2y)^\alpha}{3^\alpha} \right] & \text{for } 1 \leq t \leq \frac{4}{3} \end{cases} \quad (23)$$

where $x = x(t) \equiv \sqrt{1 - \frac{2}{3}t}$ and $y = y(t) \equiv \sqrt{1 - \frac{3}{4}t}$. Furthermore, from theorem 8 it follows that for $0 < \alpha < 2$, $\tilde{E}_{\min}^{(\alpha)}(t)$ is given by the exact same expression as in Eq.(23).

Note that $E_{\max}^{(\alpha)}(t)$ and $E_{\min}^{(\alpha)}(t)$ are continuous at the point $t = 4/3$ (i.e. $x = 1/3$ and $y = 0$), but not their derivatives. Nevertheless, since the derivatives of $E_{\max}^{(\alpha)}(t)$ and $E_{\min}^{(\alpha)}(t)$ in both regions $1 < t < 4/3$ and $3/4 < t < 3/2$ are positive, it follows that $E_{\max}^{(\alpha)}(t)$ and $E_{\min}^{(\alpha)}(t)$ are both monotonically increasing with t . Now, from Eq. (11) it follows that $t_1 + t_2 + t_3 \leq 4$ and therefore the RHS of the Eq. (22) reach its maximum value when $t_1 + t_2 + t_3 = 4$. Hence, for any $\psi \in \mathcal{H}_4$, $E_2^{(\alpha)}(\psi)$ is bounded above by ($\alpha > 2$)

$$U^{(\alpha)} \equiv \max \left\{ f_{\max}^{(\alpha)}(t_1, t_2, t_3) \mid \sum_{k=1}^3 t_k = 4, t_k \leq 3/2 \right\}.$$

Similarly, for any $\psi \in \mathcal{M}$, $E_2(\psi)$ is bounded below by ($0 < \alpha < 2$)

$$L^{(\alpha)} \equiv \min \left\{ f_{\min}^{(\alpha)}(t_1, t_2, t_3) \mid \sum_{k=1}^3 t_k = 4, t_k \leq 3/2 \right\}.$$

In Appendix C we show that $U^{(\alpha)} = f_{\max}^{(\alpha)}(4/3, 4/3, 4/3)$ and $L^{(\alpha)} = f_{\min}^{(\alpha)}(4/3, 4/3, 4/3)$. We also show that the point $t_1 = t_2 = t_3 = 4/3$ is the *only* point of global max for $f_{\max}^{(\alpha)}$ and the only point of global min for $f_{\min}^{(\alpha)}$.

Let $|\psi\rangle \in \mathcal{H}_4$, and denote by $\{P_j\}$, $\{Q_j\}$, and $\{R_j\}$ the eigenvalues of the reduced density matrices of $|\psi\rangle$ obtained after tracing out qubits C and D, B and D, and B and C, respectively. From the analysis above and the results in appendix C, $E_2^{(\alpha)}(|\psi\rangle) = U^{(\alpha)}$ if and only if $\tau_{(12)(34)}(\psi) = \tau_{(12)(34)}(\psi) = \tau_{(12)(34)}(\psi) = 4/3$ and the distributions $\{P_j\}$, $\{Q_j\}$, and $\{R_j\}$ are all of the form given in Eq.(21) with $\tau = 4/3$. That is, for $\alpha > 2$ $E_2^{(\alpha)}(|\psi\rangle) = U^{(\alpha)}$ if and only if $\{P_j\} = \{Q_j\} = \{R_j\} = \{1/3, 1/3, 1/3, 0\}$. Similarly, if $|\psi\rangle \in \mathcal{M}$ then, for $0 < \alpha < 2$, $E_2^{(\alpha)}(|\psi\rangle) = L^{(\alpha)}$ if and only if $\{P_j\} = \{Q_j\} = \{R_j\} = \{1/3, 1/3, 1/3, 0\}$.

A priori it is not clear that such a state with $\{P_j\} = \{Q_j\} = \{R_j\} = \{1/3, 1/3, 1/3, 0\}$ exists in \mathcal{H}_4 . However, now we show that up to local unitaries there exists exactly one state with this property and the state is $|L\rangle$.

First note that if $\{P_j\} = \{Q_j\} = \{R_j\} = \{1/3, 1/3, 1/3, 0\}$ then up to local unitaries $|\psi\rangle \in \mathcal{M} \subset \mathcal{A}$. Therefore, we can write $|\psi\rangle = z_0 u_0 + z_1 u_1 + z_2 u_2 + z_3 u_3$. In this case, the eigenvalues of the reduced density matrices are given by ($j = 0, 1, 2, 3$):

$$P_j = |z_j|^2, \quad Q_j = \left| \sum_{k=0}^3 A_{jk} z_k \right|^2, \quad R_j = \left| \sum_{k=0}^3 B_{jk} z_k \right|^2, \quad (24)$$

where A_{jk} and B_{jk} are the matrix element of the two orthogonal 4×4 orthogonal matrices:

$$A = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \quad \text{and} \quad B = \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}.$$

Now, since $\{P_j\} = \{1/3, 1/3, 1/3, 0\}$ we have

$$z_0 = 0, \quad z_1 = \frac{1}{\sqrt{3}} e^{i\theta_1}, \quad z_2 = \frac{1}{\sqrt{3}} e^{i\theta_2}, \quad z_3 = \frac{1}{\sqrt{3}} e^{i\theta_3},$$

where we have used the fact that the transformation $|\psi\rangle \rightarrow |\psi'\rangle = \sum_{j=0}^3 z_{\sigma(j)} u_j$ can be achieved by local unitaries for all permutations σ . With these values for z_j we get

$$\begin{aligned} Q_0 = R_0 &= \frac{1}{12} |e^{i\theta_1} + e^{i\theta_2} + e^{i\theta_3}|^2 \\ Q_1 = R_1 &= \frac{1}{12} |-e^{i\theta_1} + e^{i\theta_2} + e^{i\theta_3}|^2 \\ Q_2 = R_2 &= \frac{1}{12} |e^{i\theta_1} - e^{i\theta_2} + e^{i\theta_3}|^2 \\ Q_3 = R_3 &= \frac{1}{12} |e^{i\theta_1} + e^{i\theta_2} - e^{i\theta_3}|^2. \end{aligned} \quad (25)$$

Thus, $\{Q_j\} = \{R_j\} = \{1/3, 1/3, 1/3, 0\}$ if and only if up to permutation $e^{i\theta_1} = \pm 1$, $e^{i\theta_2} = \pm e^{i\pi/3}$, and $e^{i\theta_3} = \pm e^{i2\pi/3}$. From proposition 2 it follows that up to local unitaries $|\psi\rangle = |L\rangle$. \square

B. The State $|M\rangle$

In this section we show that the state $|M\rangle$ in Eq. (2) has the remarkable property that it *maximizes* the average Tsallis entropy of entanglement $E_2^{(\alpha)}$ for *all* $0 \leq \alpha \leq 2$. In addition, among all the states in \mathcal{M} , the state $|M\rangle$ *minimizes* $E_2^{(\alpha)}$ for *all* $\alpha \geq 2$.

Theorem 10. (a) *Let $\psi \in \mathcal{A}$. Then,*

$$E_2^{(\alpha)}(\psi) \leq E_2^{(\alpha)}(|M\rangle) \quad \text{for } 0 < \alpha < 2 \quad (26)$$

with equality if and only if up to local unitaries $\psi = |M\rangle$.

(b) *Let $\psi \in \mathcal{M}$. Then,*

$$E_2^{(\alpha)}(\psi) \geq E_2^{(\alpha)}(|M\rangle) \quad \text{for } \alpha > 2 \quad (27)$$

with equality if and only if up to local unitaries $\psi = |M\rangle$.

Proof. Let $\psi \in \mathcal{A}$, and denote $z_j \equiv \sqrt{p_j} e^{i\theta_j}$ for $j = 0, 1, 2, 3$. With this notations, $\mathcal{E}_1(\psi) = \sum_{j=0}^3 p_j e^{i2\theta_j}$, and for a fixed value of $|\mathcal{E}_1| \equiv a$, ($a \geq 0$), the formula in Theorem 6 can be written as

$$t_1(\psi) + t_2(\psi) + t_3(\psi) = 4 - a^2.$$

Moreover, note that if $|\mathcal{E}_1(\psi)| = a$ then $p_j \leq (1+a)/2$ for all $j = 0, 1, 2, 3$. Therefore, we denote by $\tilde{E}_{\max}^{(\alpha)}(a, t)$, the maximum value $E_T^{(\alpha)}(\varphi)$ can take among all normalized bipartite states $\varphi \in \mathbb{C}^4 \otimes \mathbb{C}^4$ with tangle $\tau(\varphi) = t$ and Schmidt coefficients $p_j \leq (1+a)/2$.

Now, a simple calculation shows that for a distribution of the form $p_0 \geq p_1 = p_2 = p_3$, we get that $p_j \leq (1+a)/2$ if and only if $t \geq 2(1-a)(2+a)/3$. Therefore, from theorem 8 it follows that this is the optimal distribution for $t \geq 2(1-a)(2+a)/3$. On the other hand, if $t < 2(1-a)(2+a)/3$, the optimal distribution (up to permutation) is given by $p_0 = \frac{1+a}{2} \geq p_1 \geq p_2 = p_3$. This follows from the extension of the results in [31], and in particular [32], it is a consequence of Eq.(22) in [31]. Hence, we conclude that for $0 < \alpha < 2$

$$\tilde{E}_{\max}^{(\alpha)}(a, t) = \frac{1}{\alpha - 1} \begin{cases} \left[1 - \frac{3(1-x)^\alpha}{4^\alpha} - \frac{(1+3x)^\alpha}{4^\alpha} \right] & \text{for } t \geq \frac{2(1-a)(2+a)}{3} \\ \left[1 - \left(\frac{1+a}{2}\right)^\alpha - \frac{(1-a+2\omega)^\alpha}{6^\alpha} - \frac{2(1-a-\omega)^\alpha}{6^\alpha} \right] & \text{otherwise} \end{cases} \quad (28)$$

where $x = x(t) \equiv \sqrt{1 - \frac{2}{3}t}$ and $\omega \equiv \omega(t) \equiv \sqrt{4 - 2a - 2a^2 - 3t}$.

Similar to the definition in theorem 9, we define

$$f_{\max}^{(\alpha)}(a, t_1, t_2, t_3) \equiv \frac{1}{3} \left(\tilde{E}_{\max}^{(\alpha)}(a, t_1) + \tilde{E}_{\max}^{(\alpha)}(a, t_2) + \tilde{E}_{\max}^{(\alpha)}(a, t_3) \right). \quad (29)$$

We therefore have for $0 < \alpha < 2$

$$E_2^{(\alpha)}(\psi) \leq f_{\max}^{(\alpha)}(a, t_1, t_2, t_3).$$

A straightforward calculation, similar to the one given in Appendix C, shows that the global maximum of the function $f_{\max}^{(\alpha)}(a, t_1, t_2, t_3)$ is unique and is obtained at the point $a = 0$ (i.e. $\psi \in \mathcal{M}$) and $t_1 = t_2 = t_3 = 4/3$. Therefore, from theorem 8 (and in particular from Eq. (20) with $\tau = 4/3$), it follows that this global maximum is obtained if and only if

$$P_j, Q_j, R_j \in \left\{ \frac{1}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6} \right\} \quad \forall j = 0, 1, 2, 3, \quad (30)$$

where the sets $\{P_j\}$, $\{Q_j\}$, and $\{R_j\}$ are the eigenvalues of the reduced density matrices of ψ obtained after

tracing out qubits C and D, B and D, and B and C, respectively. A priori, it is not clear that a four qubits state with these properties exists. We show now that there exists only one state (up to local unitaries) with these properties, and it is the state $|M\rangle$. Note also that if such a ψ exists then $\psi \in \mathcal{M} \subset \mathcal{A}$.

Up to a local unitary (see proposition 3), w.l.o.g. we can assume that $P_0 = 1/2$ and $P_1 = P_2 = P_3 = 1/6$. Further, due to the freedom of global phase, we have

$$z_0 = \frac{1}{\sqrt{2}}, z_1 = \frac{1}{\sqrt{6}}e^{i\theta_1}, z_2 = \frac{1}{\sqrt{6}}e^{i\theta_2}, z_3 = \frac{1}{\sqrt{6}}e^{i\theta_3}.$$

Next, the condition that three of the Q_j s and three of the R_j s equal to $1/6$ implies that $|\psi\rangle$ equals to one of the 8 states:

$$\frac{1}{\sqrt{2}}u_0 \pm \frac{i}{\sqrt{6}}u_1 \pm \frac{i}{\sqrt{6}}u_2 \pm \frac{i}{\sqrt{6}}u_3$$

Using proposition 3 we get that all these eight states are equivalent under local unitaries. We are therefore left with one state

$$\psi = \frac{1}{\sqrt{2}}u_0 + \frac{i}{\sqrt{6}}u_1 + \frac{i}{\sqrt{6}}u_2 + \frac{i}{\sqrt{6}}u_3 \quad (31)$$

Up to a local unitary, this state is the same as $|M\rangle$ in Eq. (2).

The proof of part (b) of the theorem follows the same lines as above with $a = 0$ and $\alpha > 2$. \square

C. The cluster states

We are now ready to analyze the maximally entangled states in \mathcal{M} for which two of the tangles $\{\tau_{(AB)(CD)}, \tau_{(AC)(BD)}, \tau_{(AD)(BC)}\}$ equal to the maximal value of $3/2$ while the remaining tangle equals to 1.

Theorem 11. *Let $|\psi\rangle \in \mathcal{A}$, and denote by $\{P_j\}$, $\{Q_j\}$, and $\{R_j\}$ the eigenvalues of the reduced density matrices of $|\psi\rangle$ obtained after tracing out qubits C and D, B and D, and B and C, respectively. If the Shannon entropies $H(\{P_i\}) = H(\{Q_i\}) = 2$, then $H(\{R_i\}) \leq 1$, with equality if and only if up to a local unitary $|\psi\rangle = |C_2\rangle \in \mathcal{M}$.*

Note that from the theorem above it follows that, up to a local unitary, $|\psi\rangle = |C_1\rangle$ ($|\psi\rangle = |C_3\rangle$) if one replace the condition $H(\{P_i\}) = H(\{Q_i\}) = 2$ with $H(\{Q_i\}) = H(\{R_i\}) = 2$ ($H(\{P_i\}) = H(\{R_i\}) = 2$).

Proof. Let $|\psi\rangle \in \mathcal{A}$, and define two orthogonal 4×4 orthogonal matrices:

$$A = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \text{ and } B = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 \end{pmatrix}.$$

The eigenvalues of the reduced density matrices are given by ($j = 0, 1, 2, 3$):

$$P_j = |z_j|^2, \quad Q_j = \left| \sum_{k=0}^3 A_{jk} z_k \right|^2, \quad R_j = \left| \sum_{k=0}^3 B_{jk} z_k \right|^2.$$

Hence, the equality $H(\{P_i\}) = 2$ leads to

$$z_j = \frac{1}{2}e^{i\theta_j}, \quad j = 0, 1, 2, 3.$$

Now, since a quantum state is defined up to a global phase, w.l.o.g. we can take $\theta_0 = -\theta_1$ which reduces the number of free parameters to 3. Next, the condition $H(\{Q_j\}) = 2$ together with proposition 2 implies that up to a local unitary

$$|\psi\rangle = \frac{1}{2}u_0 - \frac{1}{2}u_1 + \frac{e^{i\gamma}}{2}u_2 + \frac{e^{i\gamma}}{2}u_3,$$

where γ is the only free real parameter left. Now, it is a simple calculation to check that at least two of the R_j ($j = 0, 1, 2, 3$) equals to zero. Therefore, $H(\{R_j\}) \leq 1$. If we require that $H(\{R_j\}) = 1$, then $e^{i\gamma} = \pm i$ and up to a local unitary $|\psi\rangle = |C_2\rangle$. \square

Next we show that the three cluster states are the only states (up to local unitaries) that maximize the average Renyi entropy of degree $\alpha \geq 2$.

1. *Cluster states are the only states that maximize the average Renyi entropy with $\alpha \geq 2$*

Theorem 12. *Let $\psi \in \mathcal{H}_4$ and $\alpha \geq 2$. Then,*

$$E_2^{(\alpha)}(\psi) \leq 5/3,$$

with equality if and only if, up to local unitaries, ψ is one of the cluster states given in Eqs. (3,4,5).

Proof. We first prove it for the case $\alpha = 2$. In this case, the Renyi entropy of degree 2 (which also called collision entropy) can be expressed in terms of the linear entropy. This implies that the Renyi entropy of entanglement $E_R^{(\alpha=2)}$ can be expressed in terms of the tangle:

$$E_R^{(\alpha=2)}(|\psi^{AB}\rangle) = -\log \left(1 - \frac{1}{2}\tau(|\psi^{AB}\rangle) \right).$$

To simplify notations, we denote by t_1 , t_2 and t_3 the values of $\tau_{(AB)(CD)}(\psi)$, $\tau_{(AC)(BD)}(\psi)$, and $\tau_{(AD)(BC)}(\psi)$, respectively. With these notations we have

$$E_2^{(\alpha=2)}(\psi) = -\frac{1}{3} \log \left[\left(1 - \frac{1}{2}t_1 \right) \left(1 - \frac{1}{2}t_2 \right) \left(1 - \frac{1}{2}t_3 \right) \right]$$

Note that since $\tau_2 \leq 4/3$ we have $t_1 + t_2 + t_3 \leq 4$. Now, the function $-\log(1 - t/2)$ increase with t . Therefore,

$E_2^{\alpha=2}$ obtains its maximum value when $t_1 + t_2 + t_3 = 4$. Now, we define

$$f(t_1, t_2) \equiv \left(1 - \frac{1}{2}t_1\right) \left(1 - \frac{1}{2}t_2\right) \left(\frac{t_1 + t_2}{2} - 1\right)$$

on the domain

$$D = \{(t_1, t_2) | 1 \leq t_1 \leq 3/2, 5/2 - t_1 \leq t_2 \leq 3/2\}.$$

A simple analysis of the function $f(t_1, t_2)$ implies that $f(t_1, t_2)$ obtains its minimum value of $1/32$ only at the points $(1, 3/2)$, $(3/2, 1)$, and $(3/2, 3/2)$. Therefore, for states with these values for t_1 , t_2 and $t_3 = 4 - t_1 - t_2$, $E_2^{(\alpha=2)}$ obtains its maximum value. In theorem 11 we have seen that the 3 cluster states are the only ones with these values of t_1 , t_2 , and t_3 . This completes the proof of the theorem for $\alpha = 2$. The case for $\alpha > 2$ follows immediately from the fact that the Renyi entropy is a non-increasing function of α and therefore $E_2^{(\alpha=2)} \geq E_2^{(\alpha>2)}$. To complete the proof, we observe that for the cluster states $E_2^{(\alpha)} = 5/3$ for all α . \square

V. MORE MAXIMALLY ENTANGLED 4-QUBITS STATES

In this section we characterize all the states in $\psi \in \mathcal{A}$ that maximize the average α -entropy of entanglement $E_2^{(\alpha)}$ (as defined in Eq.(19)), for given values of $\tau_{(AB)(CD)}$, $\tau_{(AC)(BD)}$, and $\tau_{(AD)(BC)}$. We also characterize the states in \mathcal{M} for which one of the three tangles $\tau_{(AB)(CD)}$, $\tau_{(AC)(BD)}$, and $\tau_{(AD)(BC)}$, is equal to $3/2$.

We start with a definition of a class \mathcal{C} of maximally entangled states:

$\mathcal{C} \equiv$

$$\left\{ \sqrt{p}e^{i\theta}u_0 + \sqrt{\frac{1-p}{3}} \sum_{j=1}^3 u_j \mid \frac{1}{2} \leq p \leq 1, \cos^2 \theta \leq \frac{1-p}{3p} \right\}$$

Proposition 13. *Up to local unitaries, the class \mathcal{C} consists of all the states in \mathcal{A} such that all three distributions $\{P_j\}$, $\{Q_j\}$, and $\{R_j\}$, as defined in Eq. (24), have the form $\{p_0, p_1, p_1, p_1\}$ with $p_0 > p_1$; i.e. they are of the form given in Eq.(20).*

Remark. Note that the state $|M\rangle$ belongs to \mathcal{C} . It corresponds to $\theta = \pi/2$ and $p = 1/2$.

Proof. Let $\psi = z_0u_0 + z_1u_1 + z_2u_2 + z_3u_3$ be a state in \mathcal{A} with the properties mentioned in the proposition. Therefore, since $P_j = |z_j|^2$, up to local unitaries

$$\psi = \sqrt{p}u_0 + \sqrt{\frac{1-p}{3}} \sum_{j=1}^3 e^{i\theta_j} u_j,$$

with $p \geq 1/2$. From the definitions of $\{Q_j\}$ and $\{R_j\}$ in Eq. (24), and from the requirement that three of the Q_j s

are equal and smaller than $1/6$ and also three of the R_j s are equal and smaller than $1/6$, we get that $\theta_1 = \theta_2 = \theta_3 \equiv \theta$, and $\cos^2 \theta \leq (1-p)/3p$. Therefore, up to a global phase $\psi \in \mathcal{C}$. \square

Corollary 14. *Let $\psi \in \mathcal{H}_4$ and $\phi \in \mathcal{C}$. If*

$$\begin{aligned} \tau_{(AB)(CD)}(\psi) &\leq \tau_{(AB)(CD)}(\phi) \\ \tau_{(AC)(BD)}(\psi) &\leq \tau_{(AC)(BD)}(\phi) \\ \tau_{(AD)(BC)}(\psi) &\leq \tau_{(AD)(BC)}(\phi), \end{aligned}$$

then

$$\begin{aligned} E_2^{(\alpha)}(\psi) &\leq E_2^{(\alpha)}(\phi) \text{ for } 0 < \alpha < 2 \\ E_2^{(\alpha)}(\psi) &\geq E_2^{(\alpha)}(\phi) \text{ for } \alpha > 2 \end{aligned} \quad (32)$$

with equalities if and only if $\phi = \psi$ up to local unitaries.

The corollary follows directly from the proposition above and from theorem 8.

Note that the corollary above also implies that for $0 < \alpha < 2$,

$$E_2^{(\alpha)}(\psi) \leq E_2^{(\alpha)}(|M\rangle),$$

for all $\psi \in \mathcal{H}_4$ with $\tau_{(AB)(CD)}(\psi)$, $\tau_{(AC)(BD)}(\psi)$, and $\tau_{(AD)(BC)}(\psi)$ all being no greater than $4/3$.

We end this section by classifying all the states in \mathcal{M} for which one of the tangles $\tau_{(AB)(CD)}$, $\tau_{(AC)(BD)}$, and $\tau_{(AD)(BC)}$ is equal to $3/2$. Without loss of generality we will assume that $\tau_{(AB)(CD)} = 3/2$.

Proposition 15. *Let $\psi \in \mathcal{M}$. If $\tau_{(AB)(CD)}(\psi) = 3/2$ then, up to local unitaries,*

$$|\psi\rangle = \frac{1}{2}u_0 + \frac{i}{2}u_1 + \frac{e^{i\theta}}{2}u_2 + \frac{ie^{i\theta}}{2}u_3. \quad (33)$$

Remark. The two cluster states with $\tau_{(AB)(CD)} = 3/2$ have this form with $\theta = 0$ or $\theta = \pi/2$. Among all the states of this form, the choice $\theta = \pi/4$ gives the highest value for the average entropy of entanglement, but it does not reach the average entropy of entanglement of the state $|M\rangle$ (see Fig. 2).

Proof. From $\tau_{(AB)(CD)} = 3/2$ we have

$$\psi = \frac{1}{2} \sum_{j=0}^3 e^{i\theta_j} u_j.$$

Now from the condition in Eq. (16), we get $\sum_{j=0}^3 e^{i2\theta_j} = 0$. This condition with the freedom of global phase leads to the form in Eq.(33). \square

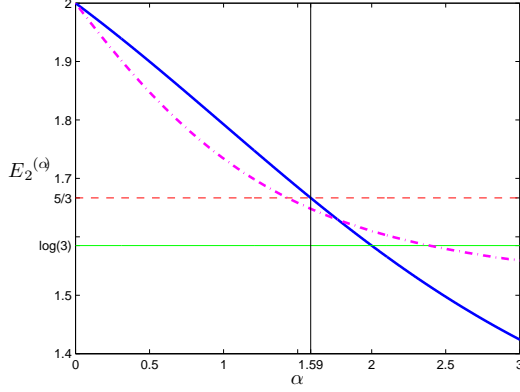


FIG. 2: A graph of the average Renyi α -entropy of entanglement as a function of α . The blue line corresponds to the state $|M\rangle$, the green line to the state $|L\rangle$, the dashed red line to the cluster states, and the dashed purple line to the state given in Eq.(33) with $\theta = \pi/4$. For $\alpha \geq 2$ we proved that the cluster states maximize $E_2^{(\alpha)}$. However, we conjecture that the cluster states maximize $E_2^{(\alpha)}$ for $\alpha > \alpha_0 \equiv 1.59\dots$ while the state $|M\rangle$ maximize it for $\alpha < \alpha_0$. Among all the states in \mathcal{M} the state $|L\rangle$ and $|M\rangle$ minimize $E_2^{(\alpha)}$ for $0 < \alpha < 2$ and $\alpha > 2$, respectively.

VI. CONCLUSIONS

Four qubits entanglement is far more complicated to analyse than its three qubits counterpart. This intricacy manifests itself with the uncountable number of inequivalent SLOCC classes. Such complexity also occur in 5 and 6 qubits systems, although for these systems there exist maximally entangled states (such as the 5-qubits code state) with the property that any bipartite cut yields a maximally entangled (bipartite) state. Since such states do not exist in 4-qubits nor in n -qubits with $n \geq 8$, the study of 4-qubits entanglement gives an insight to the structure of n -qubits maximally entangled states with large n . Indeed, some of the results presented here, such as theorem 5, can be extended to n -qubits [33].

In this paper we found an operational interpretation for the 4-tangle as a kind of 4-party residual entanglement that can not be shared between 2-qubits/2-qubits bipartite cuts. This operational interpretation enabled us to find a family of maximally entangled states that is characterized by four real parameters. All the states in the family maximize the average bipartite tangle, but only two states in the family (i.e. the states $|M\rangle$ and $|L\rangle$ in Eqs.(2,1)), maximize all the average Tsallis α -entropy of entanglement. In this sense, up to local unitary transformations, there are only two maximally entangled four qubits states.

Both the states $|M\rangle$ and $|L\rangle$ are symmetric; that is, up to local unitaries, they are both invariant under permutations of the 4 qubits. The eigenvalues of their reduced density matrices that obtained after tracing out

two qubits have the form given in Theorem 8. Therefore, since they both maximize the average bipartite tangle, we believe they also optimize many other averages of bipartite entanglement monotoness that were not introduced here. Moreover, the techniques introduced here suggest that states with the properties of $|M\rangle$ and $|L\rangle$ may exist in higher dimensional systems [33].

We also found that the three cluster states in Eqs.(3,4,5) are the only (up to local unitaries) 4-qubits states that maximize the average tangle, and have the property that out of the three reduced density matrices, that obtained by tracing out two qubits, two are proportional to the identity. In addition, we showed that the cluster states optimize the average Renyi α -entropy of entanglement with $\alpha \geq 2$. The reason that it is the cluster states and not $|M\rangle$ or $|L\rangle$ that optimize this average Renyi entropy, is that the Renyi entropy with $\alpha \geq 2$ is not concave and so the Renyi entropy of entanglement is only a deterministic entanglement monotone and *not* an ensemble monotone.

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Appendix A: Kempf-Ness Theorem

The purpose of this appendix is to state the version of the Kempf-Ness theorem that is used in this paper. Let \mathcal{H}_n be n -qubit space and let G be the subgroup $SL(2, \mathbb{C}) \otimes SL(2, \mathbb{C}) \otimes \dots \otimes SL(2, \mathbb{C})$ (n -copies) in $GL(\mathcal{H}_n)$. Let $K = SU(2) \otimes SU(2) \otimes \dots \otimes SU(2)$. Let \mathfrak{g} be the Lie algebra of G contained in $End(\mathcal{H}_n)$. We set $Crit(\mathcal{H}_n) = \{\phi \in \mathcal{H}_n \mid \langle \phi | X | \phi \rangle = 0, X \in \mathfrak{g}\}$. The Kempf-Ness theorem in this context says (the only hard part of the theorem is the “if” part of 3. which we don’t use in this paper):

Theorem 16. *Let $\phi \in \mathcal{H}_n$ then*

1. *$\phi \in Crit(\mathcal{H}_n), g \in G$ then $\|g\phi\| \geq \|\phi\|$ with equality if and only if $g\phi \in K\phi$.*
2. *If $\phi \in \mathcal{H}_n$ then $\phi \in Crit(\mathcal{H}_n)$ if and only if $\|g\phi\| \geq \|\phi\|$ for all $g \in G$.*
3. *If $\phi \in \mathcal{H}_n$ then $G\phi$ is closed in \mathcal{H}_n if and only if $G\phi \cap Crit(\mathcal{H}_n) \neq \emptyset$.*

We now assume $n = 4$. Let \mathcal{A} be as in section II. Then

Proposition 17. *$Crit(\mathcal{H}_4) = K\mathcal{A}$.*

Appendix B: Proof of theorem 8

We first prove the theorem for the von-Neumann entropy (i.e. the case $\alpha = 1$) and then we will consider the case $\alpha \neq 1$ separately. We want to optimize the function $f(\lambda_0, \lambda_1, \lambda_2, \lambda_3) = -\sum_{k=0}^3 \lambda_k \log \lambda_k$ under the

constraints $\sum_{k=0}^3 \lambda_k = 1$ and $\sum_{k=0}^3 \lambda_k^2 = 1 - \tau/2$, while $0 \leq \lambda_k \leq 1$. The Lagrangian is therefore given by

$$\mathcal{L} = -\sum_{k=0}^3 \lambda_k \log \lambda_k + \mu \left(\sum_{k=0}^3 \lambda_k - 1 \right) + \nu \left(\sum_{k=0}^3 \lambda_k^2 + \frac{\tau}{2} - 1 \right),$$

where μ and ν are the Lagrange multipliers. Therefore, the critical points in the interior of the domain (i.e. $0 < \lambda_k < 1$) must satisfy the equation:

$$\frac{\partial \mathcal{L}}{\partial \lambda_k} = -\log \lambda_k - \log e + \mu + 2\nu \lambda_k = 0 \quad (\text{B1})$$

Now, we first show that if all for λ_k satisfy the equation above, then the set $\{\lambda_k\}$ contains at most two distinct numbers. To see that, suppose that there are three distinct numbers. Then, without loss of generality, let's assume that $\lambda_0 > \lambda_1 > \lambda_2 > 0$. Thus, from the 3 equations above (for $k = 0, 1, 2$) it follows that

$$(\lambda_0 - \lambda_1) \log \lambda_2 + (\lambda_1 - \lambda_2) \log \lambda_0 = (\lambda_0 - \lambda_2) \log \lambda_1$$

Denote by $a \equiv (\lambda_1 - \lambda_2)/(\lambda_0 - \lambda_1)$. Hence, $a > 0$ and

$$\log \lambda_2 + a \log \lambda_0 = (1 + a) \log \lambda_1,$$

which is equivalent to

$$\lambda_2 \lambda_0^a = \lambda_1^{1+a}.$$

Denote by $x \equiv \lambda_2/\lambda_1$ and $y \equiv \lambda_0/\lambda_1$. Therefore, $x < 1$, $y > 1$, $a = (1 - x)/(y - 1)$, and

$$xy^a = 1.$$

From the last equation and the generalized arithmetic-geometric mean inequality we get

$$1 = (xy^a)^{1/(1+a)} \leq \frac{1}{1+a} (x + ay) = 1,$$

where the last equality is obtained by substituting $a = (1 - x)/(y - 1)$. Note that the geometric-arithmetic mean inequality is saturated if and only if $x = y$ and therefore we get a contradiction to the assumption that there are 3 distinct numbers in the set $\{\lambda_i\}$. Therefore, for the interior points we have 3 options: **(a)** $\lambda_0 \geq \lambda_1 = \lambda_2 = \lambda_3$, **(b)** $\lambda_0 = \lambda_1 \geq \lambda_2 = \lambda_3$ and **(c)** $\lambda_0 = \lambda_1 = \lambda_2 \geq \lambda_3$. Option **(b)** is the only one that does not appear in theorem 8. In this case τ must be greater than 1, and $\lambda_0 = \lambda_1 = \frac{1+\sqrt{3x(\tau)}}{4}$ and $\lambda_2 = \lambda_3 = \frac{1-\sqrt{3x(\tau)}}{4}$. It is a straightforward calculation to show that the von-Neumann entropy of this distribution never equals the von-Neumann entropy of the distributions that appear in the theorem. (Note that this is all we have to show since it has already been proved in [31] that the distributions in the theorem are the optimal ones).

As for the critical points on the boundary, set $\lambda_3 = 0$ and then the same argument as above implies that the set $\{\lambda_0, \lambda_1, \lambda_2\}$ contains at most two distinct numbers.

We therefore have two options: **(a)** $\lambda_0 = \lambda_1 \geq \lambda_2$ and **(b)** $\lambda_0 \geq \lambda_1 = \lambda_2$. Again, the distribution (b) does not appear in the theorem, but it is straightforward to show that its von-Neumann entropy never equals to the von-Neumann entropies of the distributions in the theorem. The last point on the boundary that we need to check is when $\lambda_3 = \lambda_2 = 0$, but this distribution appears in the theorem. This completes the proof for the case $\alpha = 1$.

We now prove the theorem for the case $\alpha \neq 1$ (as well as $\alpha \neq 2$). In this case, we optimize the function $f(\lambda_0, \lambda_1, \lambda_2, \lambda_3) = \sum_{k=0}^3 \lambda_k^\alpha$ under the same constraints above; that is, $\sum_{k=0}^3 \lambda_k = 1$ and $\sum_{k=0}^3 \lambda_k^2 = 1 - \tau/2$. The Lagrangian in this case is given by

$$\mathcal{L} = \sum_{k=0}^3 \lambda_k^\alpha + \mu \left(\sum_{k=0}^3 \lambda_k - 1 \right) + \nu \left(\sum_{k=0}^3 \lambda_k^2 + \frac{\tau}{2} - 1 \right),$$

where μ and ν are the Lagrange multipliers. The critical points in the interior of the domain must satisfy the equation:

$$\frac{\partial \mathcal{L}}{\partial \lambda_k} = \alpha \lambda_k^{\alpha-1} - \log e + \mu + 2\nu \lambda_k = 0 \quad (\text{B2})$$

Similarly to the argument above, we first show that the set $\{\lambda_k\}$ contains at most two distinct numbers. To see that, suppose that there are three distinct numbers $\lambda_0 > \lambda_1 > \lambda_2 > 0$. Thus, from the 3 equations above (for $k = 0, 1, 2$) it follows that

$$\frac{\lambda_0^{\alpha-1} - \lambda_1^{\alpha-1}}{\lambda_0^{\alpha-1} - \lambda_2^{\alpha-1}} = \frac{\lambda_0 - \lambda_1}{\lambda_0 - \lambda_2}.$$

Now, denote by $x \equiv \lambda_1/\lambda_0$ and $y \equiv \lambda_2/\lambda_0$. From our assumptions $0 < y < x < 1$. With these notations the equation above can be written as:

$$\frac{1 - x^{\alpha-1}}{1 - x} = \frac{1 - y^{\alpha-1}}{1 - y}.$$

However, for non-negative $\alpha \neq 2$ the function $f(x) = (1 - x^{\alpha-1})/(1 - x)$ is one-to-one and therefore we get a contradiction. This completes the proof that the set $\{\lambda_k\}$ contains at most two distinct numbers. The rest of the proof follows the same lines as the proof for the case $\alpha = 1$.

Appendix C: Global max of $f_{\max}^{(\alpha)}$ and global min of $f_{\min}^{(\alpha)}$

1. Calculation of $U^{(\alpha)}$

In this section we prove that for $\alpha > 2$, $U^{(\alpha)} = f_{\max}^{(\alpha)}(4/3, 4/3, 4/3)$, and $(4/3, 4/3, 4/3)$ is the only point of global maximum. Since the function $f_{\max}^{(\alpha)}(t_1, t_2, t_3)$ is invariant under permutations of t_1 , t_2 , and t_3 , we can assume without loss of generality that the global maximum

of $f_{\max}^{(\alpha)}$ is obtained at a point with $t_1 \geq t_2 \geq t_3$. We will therefore look for the maximum of $f_{\max}^{(\alpha)}(t_1, t_2, 4 - t_1 - t_2)$ in the domain

$$D = \left\{ (t_1, t_2) \mid \frac{4}{3} \leq t_1 \leq \frac{3}{2}, 2 - \frac{1}{2}t_1 \leq t_2 \leq t_1 \right\}.$$

In this domain, t_2 can be either bigger or smaller than $4/3$ and therefore the derivative of $f_{\max}^{(\alpha)}$ with respect to t_2 is not continuous at points with $t_2 = 4/3$. We therefore split the domain D into two regions

$$D_1 = \left\{ (t_1, t_2) \mid \frac{4}{3} \leq t_1 \leq \frac{3}{2}, \frac{4}{3} \leq t_2 \leq t_1 \right\}$$

$$D_2 = \left\{ (t_1, t_2) \mid \frac{4}{3} \leq t_1 \leq \frac{3}{2}, 2 - \frac{1}{2}t_1 \leq t_2 \leq \frac{4}{3} \right\}$$

so that on D_1 (or D_2) all the derivatives of $f_{\max}^{(\alpha)}$ are continuous. We start by maximizing $f_{\max}^{(\alpha)}$ on the domain D_1 .

a. Maximizing $f_{\max}^{(\alpha)}$ on the domain D_1

Denote by $x_i = \sqrt{1 - \frac{2}{3}t_i}$ for $i = 1, 2$ and $y = \sqrt{1 - \frac{3}{4}t_3}$. In these variables, the function $g_{\max}^{(\alpha)}(x_1, x_2) \equiv f_{\max}^{(\alpha)}(t_1, t_2, 4 - t_1 - t_2)$ is given by

$$g_{\max}^{(\alpha)}(x_1, x_2) = \frac{1}{\alpha - 1} \left[1 - \sum_{i=1,2} \left(\frac{(1+x_i)^\alpha}{4^\alpha} + \frac{1}{3} \frac{(1-3x_i)^\alpha}{4^\alpha} \right) - \frac{2}{3^{\alpha+1}}(1+y)^\alpha - \frac{1}{3^{\alpha+1}}(1-2y)^\alpha \right],$$

where in term of the variables x_1 and x_2 , $y = \frac{1}{2}\sqrt{1 - \frac{9}{2}(x_1^2 + x_2^2)}$. In terms of these new variables, the domain D_1 is given by $0 \leq x_1 \leq x_2 \leq 1/3$. We start by looking at the critical points in the interior of D_1 .

The critical points of $g_{\max}^{(\alpha)}(x_1, x_2)$ satisfies the conditions

$$\frac{\partial g_{\max}^{(\alpha)}}{\partial x_1}(x_1, x_2) = \frac{x_1}{4} (u_\alpha(y) - v_\alpha(x_1)) = 0$$

$$\frac{\partial g_{\max}^{(\alpha)}}{\partial x_2}(x_1, x_2) = \frac{x_2}{4} (u_\alpha(y) - v_\alpha(x_2)) = 0,$$

where

$$v_\alpha(x) \equiv \frac{\alpha}{(\alpha-1)4^{\alpha-1}} \frac{1}{x} [(1+x)^{\alpha-1} - (1-3x)^{\alpha-1}]$$

$$u_\alpha(y) \equiv \frac{\alpha}{(\alpha-1)3^{\alpha-1}} \frac{1}{y} [(1+y)^{\alpha-1} - (1-2y)^{\alpha-1}].$$

Hence, the point (x_1, x_2) is critical if and only if $v_\alpha(x_1) = v_\alpha(x_2) = u_\alpha(y)$, where $y = \frac{1}{2}\sqrt{1 - \frac{9}{2}(x_1^2 + x_2^2)}$ (note that $0 \leq y \leq 1/2$). In the next two lemmas we prove two useful properties of the functions $v_\alpha(x)$ and $u_\alpha(y)$.

Lemma 18. *If $2 < \alpha < 4$, and $0 \leq y \leq 1/2$, then $u'_\alpha(y) < 0$. If $2 < \alpha < 5$, and $0 \leq x \leq 1/3$, then $v'_\alpha(x) < 0$.*

Proof. A simple calculation gives

$$u'_\alpha(y) = \frac{\alpha}{(\alpha-1)3^{\alpha-1}} \frac{1}{y^2} [(1+y)^\beta(\beta y - 1) + (1-2y)^\beta(1+2\beta y)],$$

where $\beta \equiv \alpha - 2$. From the assumption of the lemma $0 < \beta < 2$. Therefore, one can easily check that $u'_\alpha(0) < 0$ and $u'_\alpha(1/2) < 0$. All that is left to show is that in the domain $0 < y < 1/2$ the function

$$w(y) \equiv (1+y)^\beta(\beta y - 1) + (1-2y)^\beta(1+2\beta y)$$

is negative. To find its maximum value, we calculate its critical points. The requirement $w'(y) = 0$ gives $(1+y)^{\beta-1} = 4(1-2y)^{\beta-1}$. Clearly, there are no critical points for $\beta \leq 1$ in the domain $(0, 1/2)$. For $\beta > 1$ we express the value of $w(y_c)$ at the critical point by substituting for $(1+y_c)^{\beta-1}$ the value $4(1-2y_c)^{\beta-1}$. This gives,

$$w(y_c) = -3(1-2y_c)^{\beta-1} [1 - 2(\beta-1)y_c] < 0,$$

for $y_c < 1/2$ and $\beta < 2$. Hence, $u'_\alpha(y) < 0$ for $2 < \alpha < 4$. Following the same arguments, one can show that $v'_\alpha(x) < 0$ for $2 < \alpha < 5$. \square

Lemma 19. *If $\alpha \geq 4$ then the global maximum of $v_\alpha(x)$ (in the domain $0 \leq x \leq 1/3$) is strictly smaller than the global minimum of the function $u_\alpha(y)$ (in the domain $0 \leq y \leq 1/2$).*

Proof. The global extremum points of u_α and v_α are obtained on the boundary or on critical points. Therefore, we first check the bounday (that is, end points). We have

$$v_\alpha(0) = \frac{\alpha}{4^{\alpha-2}}, \quad v_\alpha\left(\frac{1}{3}\right) = \frac{\alpha}{\alpha-1} \frac{1}{3^{\alpha-2}}$$

$$u_\alpha(0) = \frac{\alpha}{3^{\alpha-2}}, \quad u_\alpha\left(\frac{1}{2}\right) = \frac{\alpha}{\alpha-1} \frac{1}{2^{\alpha-2}}$$

Clearly, for $\alpha \geq 4$, we have $\max\{v_\alpha(0), v_\alpha(1/3)\} < \min\{u_\alpha(0), u_\alpha(1/2)\}$. We now estimate the values of u_α and v_α at their critical points x_c and y_c . From $u'_\alpha(y_c) = 0$ and $v'_\alpha(x_c) = 0$ we have

$$u_\alpha(y_c) = \frac{\alpha}{3^{\alpha-1}} [(1+y_c)^{\alpha-2} + 2(1-2y_c)^{\alpha-2}]$$

$$v_\alpha(x_c) = \frac{\alpha}{4^{\alpha-1}} [(1+x_c)^{\alpha-2} + 3(1-3x_c)^{\alpha-2}]. \quad (C1)$$

Since we do not have explicit expressions for x_c and y_c , we find an upper bound for $v_\alpha(x_c)$ and a lower bound for $u_\alpha(y_c)$. Since the functions in Eq. (C1) are convex for $\alpha \geq 4$, we get

$$v_\alpha(x_c) \leq \max\{v_\alpha(x_c = 0), v_\alpha(x_c = 1/3)\}$$

$$= \max\left\{\frac{1}{4} \frac{\alpha}{3^{\alpha-2}}, \frac{\alpha}{4^{\alpha-2}}\right\}$$

The minimum value of the function $u_\alpha(y_c)$ given in Eq. (C1) is obtained at the point

$$y_c = \frac{4^{1/(\alpha-3)} - 1}{1 + 2 \cdot 4^{1/(\alpha-3)}}.$$

Note that this is not necessarily the true value of y_c , but rather the value at which the function in Eq.(C1) is minimized. It is a straightforward calculation to show that at this value of y_c

$$u_\alpha(y_c) > \max \left\{ \frac{1}{4} \frac{\alpha}{3^{\alpha-2}}, v_\alpha(0), v_\alpha(1/3) \right\}.$$

This completes the proof that $u_\alpha(y) > v_\alpha(x)$ for $\alpha \geq 4$ and for all $x \in [0, 1/3]$ and $y \in [0, 1/2]$. \square

From lemma 19 it follows that for $\alpha \geq 4$ the function $g_{\max}^{(\alpha)}(x_1, x_2)$ does not have critical points in the interior of D_1 . For $2 < \alpha < 4$, $g_{\max}^{(\alpha)}(x_1, x_2)$ can have critical points. However, from the second derivatives test and from lemma 18, it follows that the Hessian is positive definite. Therefore, these critical points are local min and can not be a global max. The global maximum of $g_{\max}^{(\alpha)}(x_1, x_2)$ is therefore obtained at the boundary of D_1 .

The boundary of D_1 is a triangle with 3 sides given by $x_1 = 0$, $x_1 = x_2$, and $x_2 = 1/3$. If $x_1 = 0$ then

$$\frac{dg_{\max}^{(\alpha)}(0, x_2)}{dx_2} = \frac{x_2}{4} (u_\alpha(y) - v_\alpha(x_2)).$$

Therefore, $g_{\max}^{(\alpha)}(0, x_2)$ is convex for $2 < \alpha < 4$ (see lemma 18), and has no critical points for $\alpha \geq 4$ (see lemma 19). Therefore, its global max is obtained at one of the end points $(0, 0)$ or $(0, 1/3)$.

On the side $x_1 = x_2 \equiv x$ we have

$$\frac{d}{dx} g_{\max}^{(\alpha)}(x, x) = \frac{x}{2} (u_\alpha(y) - v_\alpha(x)).$$

Hence, the same arguments implies that the global max of $g_{\max}^{(\alpha)}(x, x)$ is obtained at one of the end points $x = 0$ or $x = 1/3$. Similarly, on the side $x_2 = 1/3$, the function $g_{\max}^{(\alpha)}(x_1, 1/3)$ obtains its global maximum at one of the end points $x_1 = 0$ or $x_1 = 1/3$. Among the three vertices $(0, 0)$, $(0, 1/3)$, $(1/3, 1/3)$, we have

$$g_{\max}^{(\alpha)}(1/3, 1/3) > \max \{ g_{\max}^{(\alpha)}(0, 0), g_{\max}^{(\alpha)}(0, 1/3) \}$$

for all $\alpha > 2$. Hence, on D_1 , $g_{\max}^{(\alpha)}$ obtains its global max at the point $(x_1, x_2) = (1/3, 1/3)$ which is equivalent to $t_1 = t_2 = t_3 = 4/3$.

b. Maximizing $f_{\max}^{(\alpha)}$ on the domain D_2

Denote by $x = \sqrt{1 - \frac{2}{3}t_1}$ and $y_i = \sqrt{1 - \frac{3}{4}t_i}$ for $i = 2, 3$. In these variables, the function $h_{\max}^{(\alpha)}(y_2, y_3) \equiv$

$f_{\max}^{(\alpha)}(4 - t_2 - t_3, t_2, t_3)$ is given by

$$h_{\max}^{(\alpha)}(y_2, y_3) = \frac{1}{\alpha - 1} \left[1 - \frac{2}{3^{\alpha+1}} \sum_{i=2,3} \left((1 + y_i)^\alpha - \frac{1}{2} (1 - 2y_i)^\alpha \right) - \frac{1}{4^\alpha} \left((1 + x)^\alpha + \frac{1}{3} (1 - 3x)^\alpha \right) \right],$$

where in term of the variables y_2 and y_3 , $x = \frac{1}{3} \sqrt{1 - 8(y_2^2 + y_3^2)}$. In terms of these new variables, the domain D_2 is therefore given by

$$D_2 = \left\{ (y_2, y_3) \mid y_2^2 + y_3^2 \leq \frac{1}{8}, y_3 \geq y_2 \geq 0 \right\}.$$

We first look at the critical points in the interior of D_2 .

The critical points of $h_{\max}^{(\alpha)}(y_2, y_3)$ satisfies the conditions

$$\begin{aligned} \frac{\partial h_{\max}^{(\alpha)}}{\partial y_2}(y_2, y_3) &= \frac{2y_2}{9} (v_\alpha(x) - u_\alpha(y_2)) = 0 \\ \frac{\partial h_{\max}^{(\alpha)}}{\partial y_3}(y_2, y_3) &= \frac{2y_3}{9} (v_\alpha(x) - u_\alpha(y_3)) = 0. \end{aligned}$$

Hence, it follows from lemma 18 and lemma 19 that the global max of $h_{\max}^{(\alpha)}(y_2, y_3)$ is obtained on the boundary of D_2 .

The boundary of D_2 consists of the line $y_2 = 0$, the line $y_1 = y_2$, and the curve $(y_2, y_3) = (\sin \theta / \sqrt{8}, \cos \theta / \sqrt{8})$ with $0 \leq \theta \leq \pi/4$. The global maximum of $h_{\max}^{(\alpha)}$ on the lines $y_2 = 0$ and $y_1 = y_2$ is obtained on one of the endpoints $(0, 1/2)$, $(0, 0)$, and $(1/4, 1/4)$. The argument follows from lemmas 18 and 19, in the same way as it was used in the analysis of the boundary of D_1 . Therefore, we focus now on the curve $(y_2, y_3) = (\sin \theta / \sqrt{8}, \cos \theta / \sqrt{8})$ with $0 \leq \theta \leq \pi/4$.

Let

$$h(\theta) \equiv h_{\max}^{(\alpha)} \left(\frac{\sin \theta}{\sqrt{8}}, \frac{\cos \theta}{\sqrt{8}} \right).$$

Note that for these values of y_2 and y_3 , $x = 0$. Hence,

$$h'(\theta) = \frac{\sin(2\theta)}{72} \left[u_\alpha \left(\frac{\cos \theta}{\sqrt{8}} \right) - u_\alpha \left(\frac{\sin \theta}{\sqrt{8}} \right) \right]$$

From lemma 18 the function u_α is one-to-one for $2 < \alpha < 4$. Therefore, the only critical point in this case is $(y_2, y_3) = (1/4, 1/4)$. For $\alpha \geq 4$ it is a simple calculation to verify that $h(\theta) < h_{\max}^{(\alpha)}(0, 0)$. Therefore, since

$$h_{\max}^{(\alpha)}(0, 0) > \max \{ h_{\max}^{(\alpha)}(1/4, 1/4), h_{\max}^{(\alpha)}(0, 1/2) \}$$

for all $\alpha > 2$, we conclude that on D_2 , $h_{\max}^{(\alpha)}$ obtains its global max at the point $(y_1, y_2) = (0, 0)$ which is equivalent to $t_1 = t_2 = t_3 = 4/3$.

2. Calculation of $L^{(\alpha)}$

In this section we prove that for $0 < \alpha < 2$, $L^{(\alpha)} = f_{\min}^{(\alpha)}(4/3, 4/3, 4/3)$, and $(4/3, 4/3, 4/3)$ is the only point of global minimum. From theorem 8 it follows that $f_{\min}^{(\alpha)}(t_1, t_2, t_3)$ for $0 < \alpha < 2$ is given by the exact same expression as $f_{\max}^{(\alpha)}(t_1, t_2, t_3)$ for $\alpha > 2$. Therefore, our proof that $L^{(\alpha)} = f_{\min}^{(\alpha)}(4/3, 4/3, 4/3)$ follows the exact same steps used in the calculation of $U^{(\alpha)}$ for $\alpha > 2$. The only difference is that the lemmas 18 and 19 do not hold for $0 < \alpha < 2$, and instead we have the following lemma.

Lemma 20. *If $0 < \alpha < 2$, $0 \leq x \leq 1/3$, and $0 \leq y \leq 1/2$, then $u'_\alpha(y) > 0$ and $v'_\alpha(x) > 0$.*

Proof. A simple calculation gives

$$u'_\alpha(y) = \frac{\alpha}{(\alpha-1)3^{\alpha-1}} \frac{1}{y^2} \left[\frac{(1+2\beta y)}{(1-2y)^\beta} - \frac{(1+\beta y)}{(1+y)^\beta} \right],$$

where $\beta \equiv 2 - \alpha$. From the assumption of the lemma $0 < \beta < 2$. Therefore, one can easily check that $\lim_{y \rightarrow 0} u'_\alpha(y) > 0$ and $\lim_{y \rightarrow 1/2} u'_\alpha(y) = +\infty$. All that is left to show is that in the domain $0 < y < 1/2$ the function

$$w(y) \equiv \frac{1}{(1-\beta)} \frac{1}{y^2} \left[\frac{(1+2\beta y)}{(1-2y)^\beta} - \frac{(1+\beta y)}{(1+y)^\beta} \right]$$

is positive. To find its minimum value, we would like to calculate its critical points. However, the requirement $w'(y) = 0$ gives $4(1+y)^{\beta+1} = (1-2y)^{\beta+1}$. Hence, there are no critical points in the domain $(0, 1/2)$. That is,, $u'_\alpha(y) > 0$ for $0 < \alpha < 2$. Following the same arguments, one can show that $v'_\alpha(x) > 0$ for $0 < \alpha < 2$. \square

With this lemma replacing lemmas 18 and 19, the proof that $L^{(\alpha)} = f_{\min}^{(\alpha)}(4/3, 4/3, 4/3)$ follows exactly the same steps that appear in the calculation of $U^{(\alpha)}$.

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 - [34] Note that f_0 is the G-concurrence [23] between qubits (1,2) and (3,4)
 - [35] A state ψ is stable if the set of states $G\psi$ is closed in \mathcal{H}_4 .
 - [36] We are willing to conjecture that it is true for all $\alpha \geq 0$.